Simulation of Liquid Crystalline Phase Transitions in Model Dipolar Systems

A. Gil-Villegas, S.C. McGrother, and G. Jackson Department of Chemistry University of Sheffield Sheffield S3 7HF, United Kingdom

The polar properties of liquid crystalline systems are of interest in applications and design of optical and measurement devices. From the theoretical and experimental points of view, molecular simulations are commonly used as important tools in improving our understanding and modeling the properties of liquid crystals. We have studied the properties of dipolar liquid crystals via Monte Carlo simulation technique for hard spherocylinders with point dipoles. In order to deal with the long-range nature of the dipole-dipole interaction we have used the reaction field method implemented with a self consistent evaluation of the dielectric constant. Our main interest has been the characterization of the phase diagram and the effects induced by the position, strength and orientation of the dipole. The main findings of our work are that for systems with central dipoles, the smectic-A (SmA) phase is stabilized relative to the nematic (N), and that ferroelectric phases are not observed. In the case of the molecules with terminal dipoles the SmA is destabilized relative to the N. Recently, we also have studied the unusual structures that the SmA phases present at very low temperature when the central dipole is transverse to the molecular axis: dipolar domains with a defined geometry (chains and loops/vortices) are observed within the plane normal to the director. These domains have some similarities with two dimensional nematic liquid crystals, and its presence suggests that the smectic phases exhibit a phase transition from a normal, free-domain, SmA to an antiferrolectric phase.